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Comparative study of the phase shift for a modified Gaussian potential by the W.K.B. method and the Eikonal method

Sachindra Nath Upadhyay
Department of Mathematics, S S College, Jiaganj-742 123, Murshidabad, India

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Abstract : Here we have considered the scattering of a nucleon in a potential field The phase shifts for a potential of the type $\frac{Ae^{-\alpha r^2}}{r}$ (modified Gaussian potential) have been calculated with the help of the W K B method The dependence of the phase shift on the values of $A/\sqrt{\alpha}$ (A being the constant of potential and α the attenuation constant) have been shown graphically The results so obtained have also been compared graphically with that of the Eikonal approximation

Keywords : Phase shift, W K B method, Eikonal approximation

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1. Introduction

The W K B. method was introduced in quantum mechanics in 1926 by Wentzel [1], Kramer [2] and Brillouin [3], although the corresponding mathematical apparatus had been developed earlier by Liouville [4], Rayleigh [5] and others. The phase shifts for the polarisation potential of the form $U(r) = \frac{-U_0}{(r^2 + d^2)^2}$ is available in the text book on quantum collision theory [6] where it is shown that for weak coupling situation ($U_0 = 1$), both the eikonal and the W.K.B. agree very well with the exact results for all values of l. But for strong coupling situation ($U_0 = 150$), the W.K.B. phase shifts are accurate for all values of l while the eikonal phase shifts are reliable only for large l-values.

In this work, we have taken the potential of the form $V = \frac{Ae^{-\alpha r^2}}{r}$ where A is the constant of potential and α is the attenuation constant (or potential decay). This form of the potential has already been assumed in the case of Eikonal approximation [7] where we have discussed the various types of potentials (mathematical models) that are generally used in the scattering problems. This is a form slightly different from the Gaussian or Yukawa form. In the case of the Eikonal approximation [7], physically tangible results may be obtained by adjusting the constants A and α. We have used the same form of the potential here so that the computed results may be compared with the earlier results for the Eikonal approximation. We shall apply the W.K.B. method to obtain the phase shift for different values of l and K and also the dependence of the phase shifts on A and α within a suitable range for the scattering of nucleon in the given potential field. Our discussion will be confined to high energy non-relativistic potential scattering so that $k/\sqrt{\alpha} \gg 1$.

2. General form of the approximation

Let us consider the scattering of a spinless particle of mass m by a real potential $V(r)$. The radial Schrödinger equation for the l-th partial wave is given by

$$\left[\frac{d^2}{dr^2} + K^2 - \frac{l(l+1)}{r^2} - U(r)\right]u_l(r) = 0, \tag{1}$$

where
$$K^2 = \frac{2mE}{\hbar^2}, \quad U(r) = \frac{2mV(r)}{\hbar^2}. \tag{2}$$

We make a change of the variable

$$r = k^{-1}e^x \tag{3}$$

and define a new unknown function $W(x)$ such that

$$u_l(r) = e^{x/2}W(x). \tag{4}$$

Then the radial Schrödinger eq. (1) becomes

$$\frac{d^2W}{dx^2} + Q^2(x)W(x) = 0, \tag{5}$$

where
$$Q^2(x) = e^{2x}(1 - U/k^2) - \left(l + \frac{1}{2}\right)^2 \tag{6}$$

Now $Q^2(x) > 0$ for x large and positive, while $Q^2(x) < 0$ when $|x|$ is large and x is negative. Then there must be a point where $Q^2(x) = 0$. Let $x = x_0$ be the turning point where $Q^2(x) = 0$ and $Q^2(x) > 0$ for $x > x_0$ and $Q^2(x) < 0$ for $x < x_0$. To solve the eq. (5) let us assume

$$W(x) = \frac{1}{\sqrt{q(x)}} \exp\left[\pm\int_{x_0}^{x} q(x')dx'\right] \tag{7}$$

to be a solution of (5), where $q(x)$ is an unknown function.

Substituting in (5) we get

$$q^2(x) + R(x) = Q^2(x), \tag{8}$$

where $$R(x) = q^{11}/2q - \frac{3}{4}(q^1)^2/q^2, \tag{9}$$

and $$q^1 = dq/dx, \; q^{11} = d^2q/dx^2.$$

The W.K.B. approximation method consists of neglecting the term $R(x)$ in the eq. (8). This is allowed provided that

$$|R(x)| \ll |Q^2(x)| \tag{10}$$

This condition will generally be fulfilled for problems where the mass is large, energy is high and the potential is smooth. We also note that for fixed values of k and l the quantity $Q^2(x)$ increases with the strength of the potential, while the correction term does not. Hence, in strong coupling limit, the W.K.B. approximation $q^2(x) = Q^2(x)$ becomes exact. Now in order to calculate the phase shift, $W(x)$ has to be constructed as smooth as possible *i.e.* it must be a continuous function with a continuous derivative for $x = -\infty$ to $x = \infty$ in both of which regions (*i.e.* on the left and right of the turning point) the eq. (7) approximates it well.

At the turning point $x = x_0$, $[Q^2(x) = 0]$, the inequality (10) is no longer valid. We shall follow here the treatment of Goldbarger and Watson [8]. We assume that in the neighbourhood of $x = x_0$, the function $Q^2(x)$ may be written as

$$Q^2(x) = \beta(x - x_0), \tag{11}$$

where β is a non-vanishing constant. This is called the linear turning point approximation. Then in the neighbourhood of $x = x_0$, the eq. (5) becomes

$$\frac{d^2w}{dy^2} + \beta y w = 0, \tag{12}$$

where $y = x - x_0$.

This equation can be integrated explicitly and we get for $x > x_0$,

$$W(x) = \frac{2D}{\sqrt{Q(x)}} \sin\left[\pi/4 + \int_{x_0}^{x} Q(x')dx'\right]. \tag{13}$$

Returning to the original variable r, we have by using the eq. (3)

$$Q^2(x) = r^2 F(r), \tag{14}$$

where $$F(r) = k^2 - U(r) - \left(l + \frac{1}{2}\right)^2 / r^2 \tag{15}$$

and the turning point $r_0 = k^{-1} \exp(x_0)$ is such that $F(r_0) = 0$.

Since $u_l(r) = [\exp(x/2)]\, W(x)$ and $\exp(x/2) = (kr)^{1/2}$, we have for $r > r_0$

$$u_l(r) = (kr)^{\frac{1}{2}} W = 2\left[k^2 / F(r)\right]^{\frac{1}{4}} D\sin\left[\frac{\pi}{4} + \int_{r_0}^{r} F^{\frac{1}{2}}(r')dr'\right]. \qquad (16)$$

To find the phase shift δ_l, we take the limit $r \to \infty$.

Now as $r \to \infty$, $F(r) \to k^2$ and we have

$$u_l(r) \to 2D\sin\left\{\frac{\pi}{4} + \int_{r_0}^{\infty}\left[F^{\frac{1}{2}}(r') - k\right]dr' + k\left(r - r_0\right)\right\}, \qquad (17)$$

where D is the constant of normalisation of the wave function. Now by comparing the eq. (17) with the asymptotic form of the radial function, namely

$$u_l(r) \underset{r\to\infty}{\to} A_l \sin(kr - l\pi/2 + \delta_l)$$

We obtain the W.K.B. phase shift

$$\delta_l(W.K.B.) = \left(l + \frac{1}{2}\right)\frac{\pi}{2} - kr_0 + \int_{r_0}^{-\infty}\left[F^{\frac{1}{2}}(r) - k\right]dr. \qquad (18)$$

3. Evaluation

Using the reduced potential

$$U(r) = \frac{A' e^{-\alpha r^2}}{r}, \quad A' = \frac{2mA}{\hbar^2}, \qquad (19)$$

we from the eq. (15)

$$F(r) = k^2 - \frac{A' e^{-\alpha r^2}}{r} - \frac{\left(l + \frac{1}{2}\right)^2}{r^2}. \qquad (20)$$

To find the phase shift from the eq. (18) we have to find out the value r_0 of r for which $F(r_0) = 0$.

Now in the integral

$$\int_{r_0}^{\infty}\left[F^{\frac{1}{2}}(r) - k\right]dr = \int_{r_0}^{\infty}\left[\left\{k^2 - \frac{A' e^{-\alpha r^2}}{r} - \frac{\left(l + \frac{1}{2}\right)^2}{r^2}\right\} - k\right]dr \qquad (21)$$

Let us put $\sqrt{\alpha r} = r'$ so that $\sqrt{\alpha r_0} = r_0'$ and eq. (21) becomes

$$\int_{r_0'}^{\infty}\left[\left\{\frac{k^2}{\alpha} - \frac{A'}{\sqrt{\alpha}}\frac{e^{-r'^2}}{r'} - \frac{\left(l + \frac{1}{2}\right)^2}{r'^2}\right\} - \frac{k}{\sqrt{\alpha}}\right]dr' \qquad (22)$$

Now, we shall find out the value of r_0' for which

$$\frac{k^2}{\alpha} - \frac{A'}{\sqrt{\alpha}}\frac{e^{-r'^2}}{r'} - \frac{\left(l+\frac{1}{2}\right)^2}{r'^2} = 0. \tag{23}$$

We measure k in units of $\sqrt{\alpha}$ and assume $\frac{A'}{\sqrt{\alpha}} = 1$,

then the eq. (23) can be written as

$$k^2 - \frac{e^{-r'^2}}{r'} = \frac{\left(l+\frac{1}{2}\right)^2}{r'^2}, \quad \text{where } k = \frac{k}{\sqrt{\alpha}} \gg 1 \tag{24}$$

or $r'^2k^2 = \left(l+\frac{1}{2}\right)^2 - r'e^{-r'^2}$, r' is small and kr' is finite of order ~ 1.

$$\left.\begin{aligned} &\text{1st approx : } r_1^2k^2 = \left(l+\frac{1}{2}\right)^2 \\ &\text{2nd approx : } r_2^2k^2 = \left(l+\frac{1}{2}\right)^2 - r_1e^{-r_1^2} \\ &\text{3rd approx : } r_3^2k^2 = \left(l+\frac{1}{2}\right)^2 - r_2e^{-r_2^2} \end{aligned}\right\} \tag{25}$$

and so on.

Thus, we find the value r_0' by successive iteration (since here k is large, r' is small and $\left(l+\frac{1}{2}\right)$ is finite). For actual evaluation, we shall continue the iteration process until we arrive at the value of r_0' which will make the difference,

$$\left| k^2 - \frac{e^{-r'^2}}{r'} - \frac{\left(l+\frac{1}{2}\right)^2}{r'^2} - 0 \right| \text{ less than } 10^{-4}.$$

Thus, we find out the value of the turning point r_0' for which the left hand side of the eq. (23) is almost equal to zero. We shall now evaluate the integral (21)

$$\int_{r_0'}^{\infty}\left[k - \left\{k^2 - \frac{e^{-r'^2}}{r'} - \frac{\left(l+\frac{1}{2}\right)^2}{r'^2}\right\}^{1/2}\right]dr'.$$

It is not possible to evaluate the integral in suitable closed form, we use numerical method [9] for the evaluation.

Let
$$R = \int_{r_0'}^{\infty} \left[k - \left\{ k^2 - \frac{e^{-r'^2}}{r'} - \frac{\left(l+\frac{1}{2}\right)^2}{r'^2} \right\}^{1/2} \right] dr'.$$

Then by applying Simpson's 1/3 rule

$$R = \frac{h}{3}\left[(I_0 + I_n) + 4\sum_{T=1}^{n/2} I_{2T-1} + 2\sum_{S=1}^{n-1} I_{2S} \right], \tag{26}$$

where h is the length of the interval and I is the value of the integrand at the corresponding points of division. Value of the integral is calculated by Simpson's (1/3) rule and we take the contribution of all the ordinates which are greater than or equal to 150-th part of the starting maximum ordinate. Substituting this value of the integral and r_0' in the eq. (18), we get the required W.K.B. phase shift.

$$\delta_l^{(\mathrm{WKB})} = \left(l + \tfrac{1}{2} \right)\pi/2 - kr_0' - R \tag{27}$$

In this way we can find out the W.K.B. phase shifts for different values of $A'/\sqrt{\alpha}$ and for different values of l and k which are plotted in Figures (1–7). We however, restrict the value

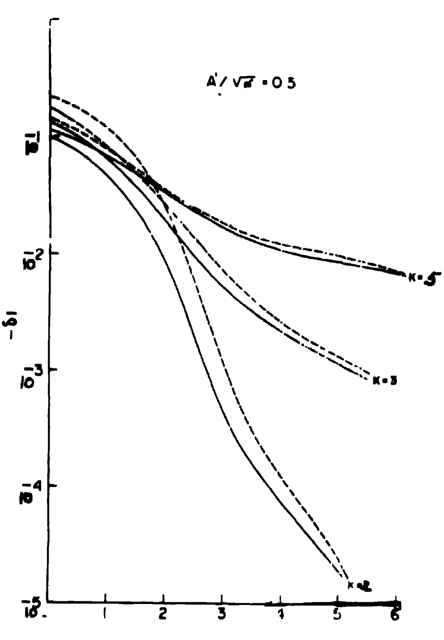

Figure 1. The phase shifts for $A'/\sqrt{\alpha}$ = 0 5 and for different values of k The solid curves represent the phase shifts for the present potential by the W K.B method and the dotted curve for that by the Eikonal method

of $A'/\sqrt{\alpha}$ upto 2, otherwise the value of r_0' obtained from eq. (24) and (25) will not hold to a good approximation.

Now, a relation between the W.K.B. and the Eikonal phase shifts can be derived [6]. For large l (and fixed k), the value of r_0' becomes large and the potential $U(r)$

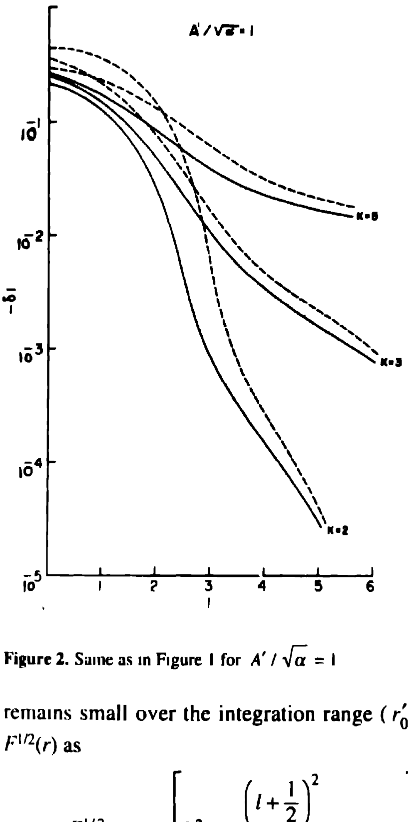

Figure 2. Same as in Figure 1 for $A'/\sqrt{\alpha} = 1$

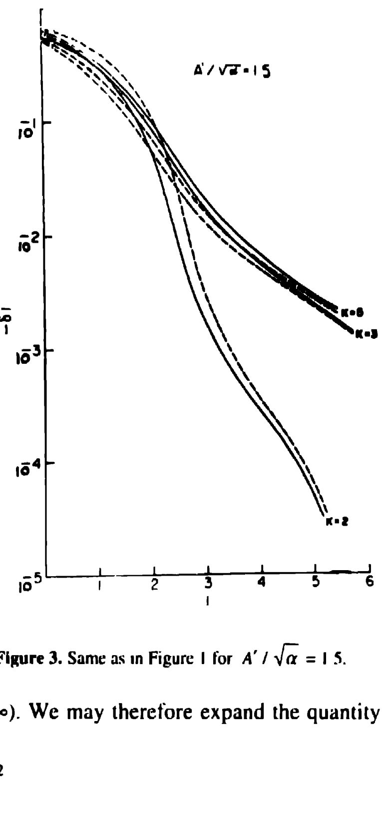

Figure 3. Same as in Figure 1 for $A'/\sqrt{\alpha} = 1.5$.

remains small over the integration range (r_0', ∞). We may therefore expand the quantity $F^{1/2}(r)$ as

$$F^{1/2}(r) = \left[k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r^2} - U(r)\right]^{1/2}$$

$$= \left[k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r^2}\right]^{1/2} \left\{1 - \frac{U(r)}{2\left[k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r^2}\right]} + \ldots\ldots\right\}, \tag{28}$$

So that we have from semi-classical approximation [6]

$$\delta_l^{(\mathrm{W.K.B.})} \simeq -\frac{1}{2k}\int_{\left(l+\frac{1}{2}\right)/k}^{\infty} \frac{rU(r)}{\left[r^2 - \left(l+\frac{1}{2}\right)^2/k^2\right]^{1/2}}\,dr, \quad \text{here } r_0 \simeq \left(l+\frac{1}{2}\right)/k$$

or
$$\delta_l^{(\mathrm{WKB})} = -\frac{1}{2k}\int_b^{\infty} \frac{rU(r)}{\sqrt{r^2-b^2}}\, dr, \tag{29}$$

where $b = \left(l+\frac{1}{2}\right)\Big/k$ the impact parameter in the Eikonal case [6].

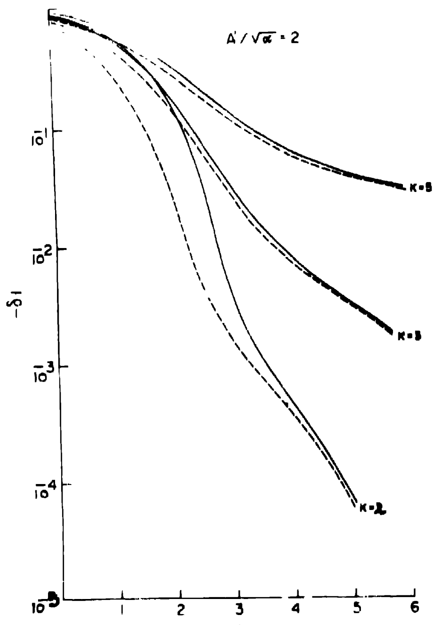

Figure 4. Same as in Figure 1 for $A'/\sqrt{\alpha} = 2$

Changing the integration variable from r to $z = \sqrt{r^2-b^2}$ and using the relation $U(b,z) = U(b,-z)$, we obtain [for large l and $\frac{k}{\sqrt{\alpha}} \gg 1$]

$$\delta_l^{(\mathrm{WKB})} \simeq -\frac{1}{4k}\int_{-\infty}^{\infty} U(b,z)dz = \frac{1}{2}\chi(k,b), \tag{30}$$

which is equal to the Eikonal phase shift. We also want to compare the W.K.B. phase shifts with that of the Eikonal phase shifts (for the same potential) which is given by [7]

$$\chi(k,b) = \frac{A'}{2k} e^{-\frac{\alpha b^2}{2}} K_0\left(\frac{\alpha b^2}{2}\right), \tag{31}$$

where K_0 is the modified Bessel function of order zero.

Now the eq. (31) can be written in the form

$$\chi(k,b) = \frac{A'/\sqrt{\alpha}}{2k/\sqrt{\alpha}} e^{-\frac{\alpha\left(l+\frac{1}{2}\right)^2}{2k^2}} K_0\left\{\frac{\alpha\left(l+\frac{1}{2}\right)^2}{2k^2}\right\}$$

or $$\chi(k,b) = \frac{-1}{2k} e^{-\frac{\left(l+\frac{1}{2}\right)^2}{2k^2}} K_0 \left\{ \frac{\left(l+\frac{1}{2}\right)^2}{2k^2} \right\}, \tag{32}$$

where similar to the W.K.B. method, we measure k in units of $\sqrt{\alpha}$ and $\frac{A'}{\sqrt{\alpha}} \sim 1$. From this equation we can calculate the Eikonal phase shift, where

$$\delta_l(k,b) = \frac{1}{2}\chi(k,b). \tag{33}$$

4. Results and discussion

With the help of the above method, we find the W.K.B. phase shifts (27) for different results of l and k as well as for different values of $\frac{A'}{\sqrt{\alpha}}$. The phase shifts for the same potential by the Eikonal method has also been calculated from the eq. (32). The results are shown in the Figures (1–4) for different values of the wave numbers (k = 2, 3, 5 in units of $\sqrt{\alpha}$) and the angular momentum quantum numbers (l = 0, 1, 2, 3, 4 and 5) and for $\frac{A'}{\sqrt{\alpha}}$ = 0.5, 1.0, 1.5 and 2.0.

where $\sqrt{\alpha} = 0.5 \times 10^{12}\,\mathrm{cm}^{-1}$

Here., k = 1, corresponds to a particle of energy 0.2 MeV.

From the Figures (1–4), we observe how the phase shift changes with the increase in the values of l and k for different values of the constant of potential. We see that for a fixed value of the constant of potential, the absolute value of the phase shift decreases with the increase in the value of l due to the centrifugal term $\frac{l(l+1)}{r^2}$ appearing in the radial equation (1), which diminishes the importance of the potential.

We also observe that the phase shifts (δ_l) by the W. K. B. method is less than that by the Eikonal method for the values of $\frac{A'}{\sqrt{\alpha}} \leq 1$ and is greater than the Eikonal method for $\frac{A'}{\sqrt{\alpha}} \geq 1$. Thus, the two curves will come closer for some value of $\frac{A'}{\sqrt{\alpha}}$ in between 1 and 2 which is reflected to some extent in the curve for $\frac{A'}{\sqrt{\alpha}}$ = 1.5. The curves for $\frac{A'}{\sqrt{\alpha}}$ = 1.5 shows that the W.K.B. curve which is below the Eikonal curve for k = 2, steadily rises and crosses it for k = 3 and k = 5. Thus, the energy dependence of the phase shifts for the two approximation are different. For higher energies, W.K.B. phase shift seems to be bigger. However, the difference between the phase shifts obtained by the two methods decreases as l increases and the results compare favourably.

In order to find out the dependence of the phase shifts on $\frac{A'}{\sqrt{\alpha}}$ by W.K.B. method, we arrange the phase shift in the following order.

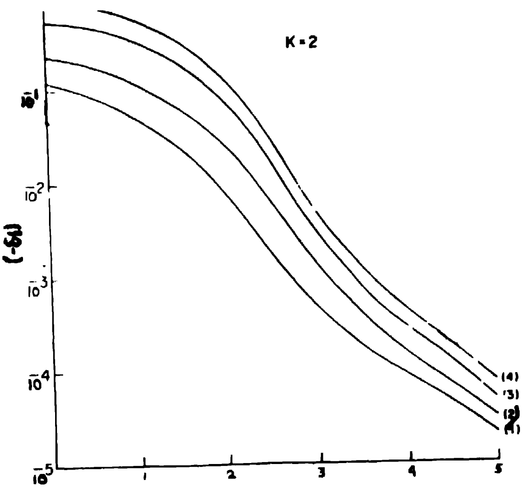

Figure 5. The phase shifts for $k = 2$ and for different values of the constant of potential *viz* (1) $A'/\sqrt{\alpha} = 0.5$, (2) $A'/\sqrt{\alpha} = 1$, (3) $A'/\sqrt{\alpha} = 1.5$, (4) $A'/\sqrt{\alpha} = 2$ by the W.K.B method

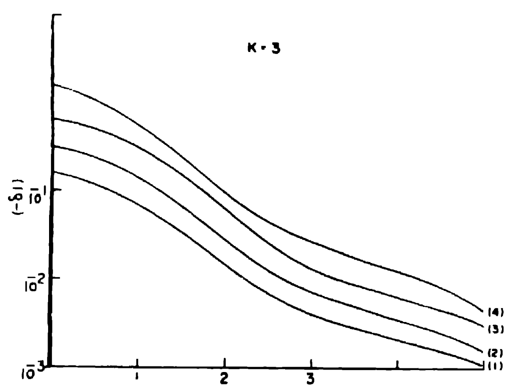

Figure 6. Same as in Figure 5 for $k = 3$.

From the Figures (5–7), we observe that with the increase in the value of the constant $\frac{A'}{\sqrt{\alpha}}$ the absolute value of the phase shift for fixed k and l increases. For a fixed $\frac{A'}{\sqrt{\alpha}}$, the value of $(-\delta_l)$ decreases with the increase in the value of l for fixed k. For a fixed $\frac{A'}{\sqrt{\alpha}}$ however, the value of $(-\delta_l)$ increases with the increase in the value of k for fixed l.

Again for a fixed $\frac{A'}{\sqrt{\alpha}}$, the decrease in the value of $(-\delta_l)$ as l increases is more rapid for lower values of k.

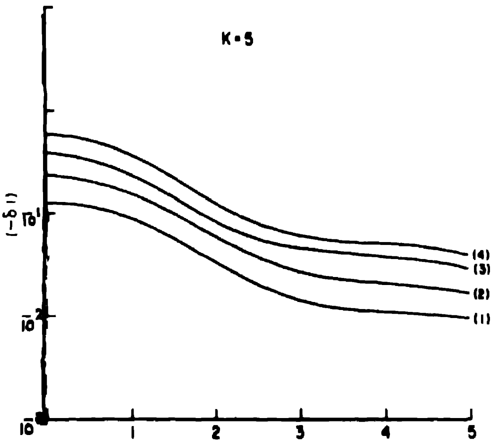

Figure 7. Same as in Figure 5 for $k = 5$

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